What is claimed is:

1. A method for detecting an impurity in a sample having at least one analyte comprising the steps of:

selecting a value representing an anticipated number of components in the sample;

generating a matrix representing characteristic measurements for the sample, said characteristic measurements having at least two variables in each dimension;

repeatedly selecting a subset within said matrix for analysis of the relation between the analyte and impurity; and

calculating an index from said subset to assess purity of the sample.

2. The method of claim 1 wherein said index represents a purity index.

3. The method of claim 1 wherein said index represents an impurity index.

4. The method of claim 1 wherein said characteristic measurements contain a baseline component.

5. The method of claim 1 wherein said characteristic measurements do not contain a baseline component.

6. The method of claim 1 wherein said characteristic measurements are spectra associated with a chromatographic peak.

7. The method of claim 3 wherein said impurity index is represented as $\boldsymbol{E}$ and calculated according to the equation:

$$\boldsymbol{E} = \sqrt{\frac{\mathbf{e}^{\mathrm{T}}\mathbf{e}}{n - r_0 - r_1}}$$

8. The method of claim 6 wherein said matrix is dimensioned with data representing retention times for the chromatographic peak and wavelengths for the spectra.

9. The method of claim 1 further comprising the step of constructing a projection matrix $\mathbf{P}_0$ by projecting each of said characteristic measurements onto said matrix to calculate a residual error.

10. The method of claim 9 further comprising the step of calculating said residual error represented by $\mathbf{e}$ according to the equation:

$$\mathbf{e} = (\mathbf{I} - \mathbf{P}_0)\mathbf{r}$$

11. The method of claim 1 wherein said subset is represented by a sub-matrix $\mathbf{R}_j$ having values which can be decomposed into the expression:

$$\mathbf{R}_j = \mathbf{U}_j\mathbf{S}_j\mathbf{V}_j^{\mathrm{T}}$$

12. The method of claim 2 wherein said purity index is represented by k_j and is calculated from $\mathbf{S}_j$ according to the equation:

$$k_j = \frac{\sum_{i=1}^{r_0+r_1} s_i}{s_r}$$

13. The method of claim 11 wherein said sub-matrix $\mathbf{R}_j$ changes its said values as it moves consecutively from one set of p columns to another such that said sub-matrix $\mathbf{R}_j$ is formed by taking the $[j$-(p-1)$/2]$ th to $[j$+(p-1)$/2]$ th column of said matrix represented by $\mathbf{R}$, for each j where $(p-1)/2+1 \geq j \geq n-(p-1)/2$.

14. An apparatus for detecting an impurity in a sample having at least one component comprising:

a device for obtaining characteristic measurements for the sample;

a computer linked to said device;

software executing on said computer for selecting a value representing an anticipated number of components in the sample;

software executing on said computer for generating a matrix representing said characteristic measurements for the sample, said characteristic measurements having at least two variables in each dimension;

software executing on said computer for repeatedly selecting a subset within said matrix for analysis of the relation between the component and impurity; and

software executing on said computer for calculating an index from said subset to assess purity of the sample.

15. The apparatus of claim 1 wherein said index represents a purity index.

16. The apparatus of claim 1 wherein said index represents an impurity index.

17. The apparatus of claim 14 wherein said characteristic measurement contains a baseline component.

18. The apparatus of claim 14 wherein said characteristic measurement does not contain a baseline component.

19. The apparatus of claim 14 wherein said characteristic measurements are spectra associated with a chromatographic peak.

20. The apparatus of claim 14 further comprising software executing on said computer for constructing a projection matrix $\mathbf{P_o}$ by projecting each of said characteristic measurements of said matrix onto said subset to calculate a residual error.

21. The apparatus of claim 14 wherein said subset is represented by sub-matrix $\mathbf{R}_j$ having values which can be decomposed into the expression:

$$\mathbf{R}_j = \mathbf{U}_j \mathbf{S}_j \mathbf{V}_j^{\mathbf{T}}$$

22. The apparatus of claim 19 wherein said matrix is dimensioned with data representing retention times for the chromatographic peak and wavelengths for the spectra.

23. The apparatus of claim 20 further comprising software executing on said computer for calculating a residual error $\mathbf{e}$ according to the equation:

$$\mathbf{e} = (\mathbf{I} - \mathbf{P}_0)\mathbf{r}$$

24. The apparatus of claim 21 wherein said sub-matrix $\mathbf{R}_j$ changes its said values as it moves consecutively from one set of p columns to another such that said sub-matrix $\mathbf{R}_j$ is formed by taking the $[j-(p-1)/2]$th to $[j+(p-1)/2]$th column of said matrix represented by $\mathbf{R}$, for each j where $(p-1)/2+1 \geq j \geq n-(p-1)/2$.

25. The apparatus of claim 20 further comprising software executing on said computer for calculating a peak impurity index represented by $\boldsymbol{E}$ according to the equation:

$$\boldsymbol{E} = \sqrt{\frac{\mathbf{e}^{\mathrm{T}}\mathbf{e}}{n - r_0 - r_1}}$$